Cooper pair formation in trapped atomic Fermi gases

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We apply the closed time-path formalism to evaluate the dynamics of the BCS transition to the superfluid state in trapped atomic ⁶Li. We find that the Fokker-Planck equation for the probability distribution of the order parameter is, sufficiently close to the critical temperature, identical to the equation that describes the switching on of a single-mode laser.

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After the successful experiments to trap and cool atomic gases of the bosonic alkalies ⁸⁷Rb, ⁷Li and ²³Na [1–3] below the critical temperature for Bose-Einstein condensation, the field of atomic physics has attracted a lot of interest. Besides the ongoing experiments on the properties of the Bose condensate in these gases, several groups have started experiments in order to observe also quantum degeneracy effects in fermionic gases. A particularly promising candidate in this respect is the fermionic isotope ⁶Li which is predicted to make a BCS transition to a superfluid state. Indeed, the triplet s-wave scattering length a_s of this atom is enormously large and negative [4], resulting in a critical temperature of the same order of those of the BEC experiments [5]. A requirement for this relatively high critical temperature is that a mixture of two different hyperfine levels of the ⁶Li atom must be trapped. Depending on the precise hyperfine states trapped, this can be done in a magnetic or optical trap. In either case, a study of the dynamics of this BCS phase transition offers the exciting opportunity to observe the evolution of a spontaneous breaking of symmetry under almost ideal conditions.

In case of a magnetically trapped gas mixture, a drawback of the large s-wave scattering length is the corresponding large decay rate and resulting limited lifetime of the gas [5,6]. Fortunately, this decay can be suppressed by applying a magnetic bias field. For example, the lifetime of a gas with a typical density of 2×10^{12} cm⁻³ atoms per hyperfine state, is of the order of 1 second in a magnetic bias field of about 7 T, whereas it is of the order of only 0.2 ms at 0.1 T. Evidently, the lifetime of the gas must be longer than the time scale on which the formation of Cooper pairs occurs. In previous work [5], we estimated on basis of mean-field theory the nucleation time to be $O(\hbar/k_BT_c)$. For a homogeneous mixture with a density of $2\times 10^{12}~{\rm cm}^{-3}$ in each hyperfine level, the critical temperature was calculated to be 37 nK, resulting in a nucleation time of 0.2 ms. Since low magnetic fields are experimentally much more convenient, it is also from this point of view sensible to make a precise calculation of the nucleation time of the BCS transition. The aim of the present paper is therefore to evaluate the dynamics of the BCS phase transition, from which, as a byproduct, the time scale for the formation of Cooper pairs can be extracted.

The dynamics of the phase transition can be described by using the closed time-path formalism [7]. This can easily be understood from an analogy in quantum mechanics where the probability amplitude for a particle moving from a position \mathbf{x}_0 at time t_0 to another position \mathbf{x} at time t is given by $\langle \mathbf{x}, t | \mathbf{x}_0, t_0 \rangle = \int \mathcal{D}[\mathbf{x}] \exp{(i\mathcal{A}[\mathbf{x}]/\hbar)}$ with $\mathcal{A}[\mathbf{x}] = \int_{t_0}^t dt' \mathcal{L}[\mathbf{x}, \dot{\mathbf{x}}]$ the action and \mathcal{L} the lagrangian of the particle. The probability distribution for being at position \mathbf{x} at time t, i.e., $P[\mathbf{x}, t] = \int d\mathbf{x}_0 \langle \mathbf{x}, t | \mathbf{x}_0, t_0 \rangle \langle \mathbf{x}_0, t_0 | \mathbf{x}, t \rangle P[\mathbf{x}_0, t_0]$, is now given by a path integral over the periodic paths $[\mathbf{x}(t')]$ where t' runs from t to t_0 (antichronological, lower branch) and back from t_0 to t (chronological, upper branch), i.e., over a closed time or Keldysh contour [7,8].

In our case, we want to study the dynamics of the BCS phase transition. Analogous to the simple quantum mechanical description for the position probability of a particle, we thus need to derive the time dependence of the probability distribution for the order parameter Δ which describes the superfluid phase [9–11]. The starting point is the probability $P[\psi, \psi^*, t]$ for a gas of atoms in two hyperfine states denoted by $|\alpha\rangle = |\uparrow\rangle, |\downarrow\rangle$

$$P[\psi, \psi^*, t] = \int \mathcal{D}[\psi] \mathcal{D}[\psi^*] \exp\left(\frac{\imath}{\hbar} \mathcal{A}[\psi, \psi^*]\right)$$

where the functional integral is over the fermionic fields $\psi_{\alpha}(\mathbf{x},t)$ and $\psi_{\alpha}^{*}(\mathbf{x},t)$ that are defined on the Keldysh contour C with $t_{0} \to -\infty$. The action $\mathcal{A}[\psi,\psi^{*}]$ is given by

$$\mathcal{A}[\psi, \psi^*] = \sum_{\alpha} \int_{C} dt \int d\mathbf{x} \psi_{\alpha}^*(\mathbf{x}, t) \left(i\hbar \frac{\partial}{\partial t} + \frac{\hbar^2 \nabla^2}{2m} + \mu_{\alpha} - \frac{V_0}{2} \psi_{-\alpha}^*(\mathbf{x}, t) \psi_{-\alpha}(\mathbf{x}, t) \right) \psi_{\alpha}(\mathbf{x}, t),$$

where $V_0 < 0$ represents a local attractive interatomic interaction. Introducing by means of a Hubbard-Stratonovich transformation the order parameter $\Delta(\mathbf{x},t)$, the action becomes quadratic in the fermionic fields and ψ and ψ^* can easily be integrated out [10]. We thus arrive at an effective field theory for this order parameter $\Delta(\mathbf{x},t)$ that equals

$$\mathcal{A}[\Delta, \Delta^*] = -i\hbar \text{Tr}[\ln G^{-1}] + \int_C dt \int d\mathbf{x} \frac{|\Delta(\mathbf{x}, t)|^2}{V_0}, \quad (1)$$

where the trace runs over the spin, time and spatial variables, and the Green's function matrix is defined as $G(\mathbf{x},t;\mathbf{x}',t') \equiv -\imath \langle T_C[\psi(\mathbf{x},t)\psi^*(\mathbf{x}',t')] \rangle$. The spinor $\psi^*(\mathbf{x},t)$ is given by $\psi^*(\mathbf{x},t) \equiv \left(\psi^*_{\downarrow}(\mathbf{x},t), \psi_{\uparrow}(\mathbf{x},t)\right)$ and T_C is the time ordening operator on the Keldysh contour C, taking into account the anti-commuting nature of the fields.

Around the critical temperature T_c , the order parameter Δ is small compared to k_BT , and Eq. (1) can be expanded in powers of Δ . To include to lowest order all relevant physics, it suffices to take only the terms proportional to $|\Delta|^2$ and $|\Delta|^4$ into account. To calculate these quadratic and quartic parts of the effective action for Δ explicitly, we must remember that the time integrals within these expressions are over the Keldysh contour, and must be rewritten as time integrals over the real axis $-\infty < t' < t$ only. The Green's function $G_0(\mathbf{x}, t; \mathbf{x}', t')$ defined on the contour, must then be decomposed into retarded, advanced and Keldysh components. Furthermore, the order parameter $\Delta(\mathbf{x}, t)$ on the contour can be decomposed in a classical part ϕ and fluctuations ξ defined on the real time axis as

$$\Delta(\mathbf{x}, t_{\pm}) = \phi(\mathbf{x}, t) \pm \frac{1}{2} \xi(\mathbf{x}, t)$$

where the upper and lower sign refer to the upper and lower branch of the Keldysh contour, respectively. The important point is that the fluctuations allow the classical part of the order parameter to evolve from zero to a nonzero value when the system is driven through the phase transition, and we can thus indeed describe the dynamics of the classical field ϕ around the critical temperature by means of this closed time-path method. In contrast, this cannot be achieved within the framework of mean-field theory, where the order parameter always remains zero if it is zero initially.

Applying subsequently a gradient expansion which assumes that spatial and temporal variations in the order parameter are small on the size of the Cooper pairs, the quadratic plus quartic part of the effective action Eq. (1) up to quadratic order in the fluctuations, becomes

$$\mathcal{A}[\phi, \phi^*, \xi, \xi^*] = \int d\mathbf{x} \int_{-\infty}^t dt' \left\{ \phi(\mathbf{x}, t') L^{(R)}(\mathbf{x}, t') \xi^*(\mathbf{x}, t') + \xi(\mathbf{x}, t') L^{(A)}(\mathbf{x}, t') \phi^*(\mathbf{x}, t') + \frac{1}{2} \xi(\mathbf{x}, t') L^{(K)}(\mathbf{x}, t') \xi^*(\mathbf{x}, t') \right\},$$
(2)

where to lowest non-vanishing order in ∇ and in $\partial/\partial t$ the retarded and advanced factors are [9,10]

$$L^{(R,A)}(\mathbf{x},t) = \alpha + \gamma \nabla^2 - \beta |\phi(\mathbf{x},t)|^2 \pm N_0 \frac{\pi}{8} \frac{\hbar}{k_B T} \frac{\partial}{\partial t}$$
(3)

and the Keldysh part is given by

$$L^{(K)}(\mathbf{x},t) = iN_0 \frac{\pi}{2}.\tag{4}$$

Here we considered only the optimal case $\mu_{\uparrow} = \mu_{\downarrow}$ and used particle-hole symmetry around the Fermi level of the system. The constants α , β and γ are given by

$$\alpha = N_0 \left(1 - \frac{T}{T_c} \right) \tag{5}$$

$$\beta = N_0 \frac{7}{8} \frac{\zeta(3)}{(\pi k_B T)^2} \tag{6}$$

$$\gamma = N_0 \frac{7}{8} \frac{\zeta(3)}{6\pi^2} \left(\frac{\hbar v_F}{k_B T}\right)^2. \tag{7}$$

Furthermore, $N_0 = mk_F/(2\pi^2\hbar^2)$ denotes the density of states at the Fermi level, the critical temperature obeys $k_BT_c \simeq 5/3\epsilon_F \exp(-1/\lambda)$ [5] with $\lambda = 2k_F|a_s|/\pi$, and v_F is the Fermi velocity of the system.

The last term in the right-hand side of Eq. (2) describes the quadratic fluctuations. If one would neglect them, and integrate out the (in that case linear) fluctuations, one would obtain a (dissipative) non-linear Schrödinger equation for the classical part ϕ of the order parameter which would also arise from equilibrium theory. Of course, for our non-equilibrium purposes, the quadratic fluctuations are important. The Fourier transforms of Eqs. (3) and (4), $L^{(R,A)}(\mathbf{k},\omega)$ and $L^{(K)}(\mathbf{k},\omega)$ in principle are related through the fluctuation-dissipation theorem

$$L^{(K)}(\mathbf{k},\omega) = \pm 2i \left(2N^B(\hbar\omega) + 1\right) \operatorname{Im}[L^{(R),(A)}(\mathbf{k},\omega)]$$
(8)

where $N^B(\hbar\omega)$ denotes the Bose distribution evaluated at $\hbar\omega$. At low frequencies it thus gives $L^{(K)}(\mathbf{k},\omega)=\pm 2i(2k_BT/\hbar\omega)\mathrm{Im}[L^{(R),(A)}(\mathbf{k},\omega)]$, in agreement with the above results. Notice that if we expand the quadratic part of the action \mathcal{A} in Eq. (1) up to lowest nonvanishing order in ∇ and $\partial/\partial t$, we only have to expand the quartic part of \mathcal{A} to zeroth order, i.e. we only need to consider the local contributions proportional to $\phi(\mathbf{x},t)\xi^*(\mathbf{x},t)|\phi(\mathbf{x},t)|^2$ and it's complex conjugate. Since the factor β has no imaginary part, we conclude that it is indeed consistent to neglect Keldysh-like terms that would in principle also arise from the quartic part of the action \mathcal{A} .

In order to arrive at an equation of motion for the probability distribution of the classical value ϕ , we first integrate out the fluctuations ξ from the action. Before doing so, we however need to realize that in real experiments, the gas will be trapped in an external potential $V_{\text{ext}}(x)$ generally in the shape of a 3D isotropic harmonic oscillator $V(x) = 1/2 m\omega_0^2 \mathbf{x}^2$. As a result, the coefficients α , β and γ in Eqs. (5) to (7) now depend on \mathbf{x} , since the Fermi energy $\mu_{\alpha}(\mathbf{x}) = \mu_{\alpha} - V(\mathbf{x}) - (4\pi a_s \hbar^2/m) n_{-\alpha}(\mathbf{x})$ and therefore the densities $n_{\alpha}(\mathbf{x})$ and the critical temperature $T_c(\mathbf{x})$ are position dependent. Hence, we can make use of the following expansion in the effective action Eq. (2) $\phi(\mathbf{x},t) = \sum_n a_n(t)\phi_n(\mathbf{x})$ and $\xi(\mathbf{x},t) = \sum_n b_n(t)\phi_n(\mathbf{x})$, where the normalized wave functions $\phi_n(\mathbf{x})$ are solutions to Schrödinger's equation [12]

$$-\left[\alpha(\mathbf{x}) + \gamma(\mathbf{x})\nabla^2\right]\phi_n(\mathbf{x}) = N_0(\mathbf{x})\varepsilon_n\phi_n(\mathbf{x}). \tag{9}$$

It is well-known that close to T_c , the spatial region where the order parameter becomes non-zero, is small compared to the region over which the density changes [5,12]. So, we can take $N_0(\mathbf{x}) \simeq N_0(\mathbf{0})$, $v_F(\mathbf{x}) \simeq v_F(\mathbf{0})$, but we must expand $T_c(\mathbf{x})$ around $\mathbf{x} = \mathbf{0}$, since it depends exponentially on the coupling constant $\lambda(\mathbf{x})$.

Considering again only the optimal case that $\mu_{\downarrow} = \mu_{\uparrow}$ and using that the density in each hyperfine level around $\mathbf{x} = \mathbf{0}$ can be approximated with $n_{\alpha}(\mathbf{x}) = 1/2 n_t(\mathbf{0})(1 - (\mathbf{x}/R)^2)$, where $n_t(\mathbf{0})$ is the total gas density in the center of the trap, one finds from the zero temperature expression for the respective chemical potentials that

$$R^2 = l^4 \left(4\pi n_t(\mathbf{0})a + 2\left(\frac{\pi^2}{\sqrt{3}}\right)^{2/3} [n_t(\mathbf{0})]^{2/3} \right),$$

where $l = \sqrt{\hbar/m\omega_0}$. From this expression one can immediately see that the effect of the mean-field interaction in the gas is to contract the gas cloud to the center of the trap. Expanding $T_c(\mathbf{x})$ around $\mathbf{x} = \mathbf{0}$, one arrives at [12]

$$\alpha(\mathbf{x}) = N_0(\mathbf{0}) \left\{ \ln \left(\frac{T_c(\mathbf{0})}{T} \frac{\epsilon_F(\mathbf{x})}{\epsilon_F(\mathbf{0})} \right) - \frac{1}{\lambda(\mathbf{0})} \left(\frac{N_0(\mathbf{0})}{N_0(\mathbf{x})} - 1 \right) \right\}$$

and Eq. (9) turns out to be just the Schrödinger equation for a 3D harmonic oscillator with effective frequency

$$\omega_{\Delta} = 4\pi \sqrt{\frac{2\lambda + 1}{7\lambda\zeta(3)}} \frac{k_B T}{m v_F(\mathbf{0}) R} \equiv \frac{\hbar}{m l_{\Delta}^2}.$$

The eigenvalues are given by

$$\varepsilon_n = \frac{2m}{\hbar^2} \frac{\gamma(\mathbf{0})}{N_0(\mathbf{0})} \left(n + \frac{3}{2} \right) \hbar \omega_\Delta - \ln \left(\frac{T_c(\mathbf{0})}{T} \right). \tag{10}$$

Notice that depending on the temperature, the eigenvalues ε_n become unstable, i.e., with decreasing temperature they can become negative one by one. The temperature where ε_0 becomes zero, is the critical temperature T_c of the inhomogeneous system. It is clear from Eq. (10) that due to finite size effects, this critical temperature T_c is lower than the homogeneous critical temperature $T_c(\mathbf{0})$ corresponding to the density in the center of the trap [12]. Now it is important to realize, that there is always a region sufficiently close to the critical temperature T_c of the system, where it is a good approximation to take into account only one single mode

$$\phi_0(\mathbf{x}) = \left(\frac{1}{\sqrt{\pi l_\Delta}}\right)^{3/2} \exp\left(-\frac{\mathbf{x}^2}{2l_\Delta^2}\right) \tag{11}$$

in the expansion for ϕ and ξ because the higher modes ϕ_n remain stable and their influence thus remains small. Furthermore, as will be shown explicitly by a numerical example later on, the coupling between modes in the nonlinear terms of Eqs. (2) and (3) can be neglected

sufficiently close to the critical temperature. Plugging everything into the action \mathcal{A} in Eq. (2), we can first perform the integral over \mathbf{x} , and subsequently integrate out the fluctuations that are now solely represented by the fields $b_0(t)$ and $b_0^*(t)$. From the resulting action the effective hamiltonian for the classical fields $a_0(t)$ and $a_0^*(t)$ can be obtained by introducing their conjugated momenta in the standard way. We find

$$H_{\Delta} = \frac{8ik_BT}{\pi N_0(\mathbf{0})} \left\{ 2k_BT \frac{\partial^2}{\partial a_0 \partial a_0^*} + \frac{\partial}{\partial a_0} [N_0(\mathbf{0})\epsilon_0 + \beta'|a_0|^2]a_0 + \frac{\partial}{\partial a_0^*} [N_0(\mathbf{0})\epsilon_0 + \beta'|a_0|^2]a_0^* \right\},$$

where $\beta' = \beta \int d\mathbf{x} |\phi_0(\mathbf{x})|^4 = \beta/(2\pi l_\Delta^2)^{3/2}$.

The equation of motion, or Fokker-Planck equation, for the probability distribution P is now given by Schrödinger's equation

$$i\hbar \frac{\partial}{\partial t} P = H_{\Delta} P \tag{12}$$

which has an equilibrium solution

$$P(a_0, a_0^*) \propto \exp\left(-\frac{V(a_0, a_0^*)}{k_B T}\right)$$

where the potential $V(a_0, a_0^*) = N_0(\mathbf{0})\epsilon_0|a_0|^2 + 1/2 \beta'|a_0|^4$. Since $\beta' > 0$, this potential has the shape of a parabolic well for $T > T_c$ where $\varepsilon_0 > 0$, whereas it becomes mexican-hat shaped below the critical temperature where $\varepsilon_0 < 0$.

The dynamics of the phase transition can most easily be extracted if we introduce dimensionless variables I, θ , τ , and the constant a according to

$$a_{0} = \left(\frac{k_{B}T}{2\beta'}\right)^{\frac{1}{4}} \sqrt{I} \exp i\theta$$

$$t = \frac{\pi N_{0}(\mathbf{0})\hbar}{\sqrt{32(k_{B}T)^{3}\beta'}} \tau$$

$$a = -\sqrt{\frac{2\beta'}{k_{B}T}} \frac{N_{0}(\mathbf{0})\epsilon_{0}}{\beta'}.$$
(13)

The Fokker-Planck equation Eq. (12) can then be rewritten in the form

$$\frac{\partial}{\partial \tau}P = \left\{ \frac{\partial^2}{\partial I^2} 4I + \frac{1}{I} \frac{\partial^2}{\partial \theta^2} + \frac{\partial}{\partial I} [2(I-a)I - 4] \right\} P \quad (14)$$

which exactly is the Fokker-Planck equation associated with the single-mode laser [13]. The constant a represents the 'pump parameter', and I is equivalent to the 'laser intensity'.

The second term on the right-hand side of Eq. (14) gives rise to phase-diffusion [14], but when the system is initially in a state which does not depend on θ , it will remain phase independent, and we can omit this term from

the Fokker-Planck equation. The stationary solution in terms of the dimensionless variables becomes

$$P_{\rm st}(I,a) = \mathcal{N}(a) \exp\left(-\frac{(I-a)^2}{4}\right),\tag{15}$$

where $\mathcal{N}(a)$ is a normalization factor. This is a Gaussian distribution centered around I=a, where a<0 for $T>T_c$, and a>0 for $T< T_c$. Note, however, that I only assumes positive values, so even above the critical temperature, the average $\langle I \rangle$ is larger than zero.

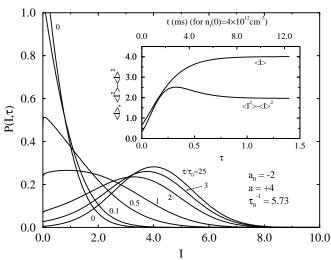


FIG. 1. Evolution of the probability distribution for the order parameter in normalized units. The inset shows the average value $\langle I \rangle$, and its variance as a function of time.

One can model the phase transition by changing the constant a suddenly from a negative value $a_0 < 0$ to a positive value a > 0 at $\tau = 0$. Indeed, the process of evaporative cooling is very fast, due to the large value of the s-wave scattering length and corresponding large cross section for elastic collisions. As a consequence, the 'translational' degrees of freedom of the atoms in the gas are always in thermal equilibrium, but the order parameter is not and needs more time to adapt. The probability distribution $P(I, \tau, a)$ will therefore evolve from the stationary solution $P_{\mathrm{St}}(I,a_0)$, see Eq. (15), at $\tau=0$ to the stationary solution $P_{\mathrm{St}}(I,a)$ at sufficiently large τ . We have solved Eq. (14) numerically for $a_0 = -2$ and a = +4using the methods developed in Ref. [13]. The evolution of the probability distribution $P(I,\tau)$ is plotted for several times in Fig. 1. It is clear that after a dimensionless time of O(1), the order parameter of the phase transition has reached its stationary value. This is shown explicitly in the inset of Fig. 1, where the average $\langle I \rangle(\tau)$ and the variance $\langle (I - \langle I \rangle)^2 \rangle (\tau)$ are plotted.

In order to see to what extent the approximations we have made are valid, we finish the paper with an explicit numerical example. For a gas mixture with density $n_{\alpha}(\mathbf{0}) = 2 \times 10^{12} \text{ cm}^{-3}$, or equivalently $n_{t}(\mathbf{0}) = 4 \times 10^{12} \text{ cm}^{-3}$, one has for the homogeneous critical temperature

 $T_c(\mathbf{0}) \simeq 37 \,\mathrm{nK}$ [5]. If this gas is trapped in a 3D isotropic harmonic oscillator with $\hbar\omega_0/k_B=7.1 \,\mathrm{nK}$ [2], the extend of the cloud is $R\simeq 11l$ at $T=30 \,\mathrm{nK}$, whereas $l_\Delta\simeq 2l$ is then indeed much smaller. The critical temperature T_c according to Eq. (10) is $T_c\simeq 31 \,\mathrm{nK}$. The second mode of Eq. (10) becomes unstable only at $T\simeq 26 \,\mathrm{nK}$. At this temperature the pump parameter $a\simeq 13$, which gives a first requirement for our theory. However, a more stringent one is that it is only a good approximation to take one single mode into account if we can also neglect the nonlinear coupling in the hamiltonian. We must then require that the interaction $\beta |\phi(\mathbf{0})|^2$ is small compared to $N_0(\mathbf{0})\hbar\omega_\Delta$. This is true for $T>29.3 \,\mathrm{nK}$, from which it follows that the approximations are valid if $a\le 4.3$. For $T=29.3 \,\mathrm{nK}$, the order parameter $\Delta(\mathbf{0})/k_BT\simeq 1$.

In Fig. 1 we therefore have chosen a = 4, and from the inset of this figure we conclude that for a total density $n_t(\mathbf{0}) = 4 \times 10^{12} \text{ cm}^{-3}$, one unit of dimensionless time τ corresponds to 8.9 ms, which is much larger than the $\hbar/k_BT_c(\mathbf{0}) = 0.2 \text{ ms as estimated in our previous work}$ [5], because Eq. (13) clearly shows that the time scale depends also on several other relevant parameters. In addition, this is caused by a critical slowing down, which can be reduced by increasing the final value of the pump parameter a, but requires inclusion of more modes in the theory. In a future publication we will come back to this multi-mode regime. However, within the present theory, for a lifetime of the gas of the order of the nucleation time, one needs a magnetic bias field of about 0.7 T. A better option is to trap and cool the lowest two hyperfine states in an optical trap, which has recently been shown to be possible for bosons [15]. In any case, we believe that this paper, in combination with Ref. [5], shows that there are no theoretical limitations to achieve a BCS transition in atomic ⁶Li.

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